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The Structure of an Organo-aluminum Ketimine Derivative [Ph2Al.N=CPh.C6H4Br]2.2C6H6

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Crystals of [Ph2Al.N=CPh.C6H4Br]2.2C6H6 are triclinic, space group $P\bar{1}$, with $Z=1$. The structure was solved by the heavy atom method and refined by least-squares to $R=10\cdot7\%$. The molecule contains a four-membered ring of alternating Al and N atoms, with Al–N = $1\cdot92$ Å, and N=C = $1\cdot28$ Å. The benzene molecules undergo large amplitude vibrations.

Introduction

Aluminum alkyls and aryls form adducts with nitriles, and on heating the adducts rearrange to give ketimine derivatives. Gibson & Hughes (1964) described the compound from triphenylaluminum and benzonitrile, and reported a degree of association in solution of $1\cdot2$–$1\cdot4$. Wade and co-workers (Lloyd & Wade, 1965; Jennings, Lloyd & Wade, 1965; Wade & Wyatt, 1967) have obtained similar compounds by the same route, and also by elimination of hydrocarbon from ketimine adducts, reporting that the compounds are dimeric.

The present work was undertaken in order to establish the degree of association and molecular structure of these compounds. Shearer & Willis (reported in Coates & Wade, 1967) have determined the structure of a related compound, [Bu^{t}MeC=N.AlMe2]2.

Mr G. K. J. Gibson kindly supplied a sample of the rearrangement product from *p*-bromobenzonitrile and triphenylaluminum. The material was recrystallized from benzene, giving a solvate containing two molecules of benzene to each dimeric molecule of the aluminum compound. Crystals were sealed in capillaries for X-ray study.

Crystal data

Al2N2C50H38Br2.2C6H6, $M=1036\cdot9$, triclinic, $a=9\cdot88$, $b=14\cdot56$, $c=9\cdot85$ Å, $\alpha=107\cdot5°,\beta=95\cdot1°$, $\gamma=99\cdot0°$, $V=1321$ Å^3. Space group $P\bar{1}$, $Z=1$, $D_x=1\cdot303$.

Structure determination

The cell dimensions were measured from zero layer precession photographs. Intensities were estimated visually from Cu $K\alpha$ Weissenberg photographs of reciprocal-lattice layers $hk0$ to $hk7$, giving 1854 independent structure amplitudes. The bromine and aluminum positions were obtained from a three-dimensional Patterson synthesis, and were consistent with the centrosymmetric space group. An electron density synthesis based on the Br and Al positions revealed the remaining non-hydrogen atoms of the molecule, but the benzene molecule appeared only as an annulus of electron density with no well-resolved peaks. After least-squares refinement of atomic positions and isotropic temperature factors a difference synthesis was

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used to locate the benzene molecule. The thermal motion of the solvent molecule was clearly very high, but peaks due to the six carbon atoms were just resolved from the annulus of electron density of the ring. Further least-squares refinement, varying atomic coordinates and anisotropic temperature factors, together with eight layer scale factors, converged to $R = 0.107$. The weighting scheme used was $w = 1/(10 + F_o + 0.02\ F_o^2)$.

Table 1. *Fractional coordinates and e.s.d.'s*

	x	y	z
Al	0·4205 (4)	0·4062 (2)	0·4122 (4)
N	0·4095 (9)	0·5421 (6)	0·4572 (10)
Br	0·3249 (2)	1·0243 (1)	0·6009 (2)
C(1)	0·3136 (12)	0·5182 (8)	0·4141 (12)
C(2)	0·3186 (11)	0·6886 (8)	0·4604 (13)
C(3)	0·2813 (13)	0·7346 (8)	0·3570 (14)
C(4)	0·2901 (14)	0·8347 (9)	0·3969 (15)
C(5)	0·3274 (14)	0·8872 (9)	0·5470 (17)
C(6)	0·3509 (15)	0·8443 (9)	0·6469 (15)
C(7)	0·3475 (14)	0·7450 (9)	0·6089 (14)
C(8)	0·1893 (12)	0·5243 (8)	0·3076 (12)
C(9)	0·0588 (13)	0·5319 (10)	0·3447 (16)
C(10)	−0·0595 (16)	0·4782 (11)	0·2529 (21)
C(11)	−0·0507 (17)	0·4124 (11)	0·1176 (21)
C(12)	0·0803 (17)	0·4080 (10)	0·0786 (17)
C(13)	0·2001 (15)	0·4602 (9)	0·1717 (14)
C(14)	0·2806 (12)	0·3304 (8)	0·4893 (13)
C(15)	0·1470 (12)	0·2933 (9)	0·4133 (14)
C(16)	0·0444 (15)	0·2362 (11)	0·4659 (18)
C(17)	0·0807 (14)	0·2209 (11)	0·5929 (19)

Table 1 (*cont.*)

	x	y	z
C(18)	0·2072 (16)	0·2569 (11)	0·6726 (17)
C(19)	0·3105 (14)	0·3136 (10)	0·6239 (14)
C(20)	0·4504 (12)	0·3470 (7)	0·2138 (13)
C(21)	0·3855 (13)	0·2508 (8)	0·1352 (12)
C(22)	0·4096 (16)	0·2056 (11)	−0·0073 (16)
C(23)	0·4937 (15)	0·2573 (12)	−0·0771 (15)
C(24)	0·5591 (14)	0·3526 (10)	−0·0008 (14)
C(25)	0·5351 (13)	0·3979 (10)	0·1401 (14)
C(26)	0·1315 (28)	0·0100 (16)	0·2274 (23)
C(27)	0·2574 (28)	0·0071 (14)	0·1939 (27)
C(28)	0·2855 (27)	−0·0580 (21)	0·0807 (29)
C(29)	0·1791 (36)	−0·1313 (23)	0·0012 (29)
C(30)	0·0502 (31)	−0·1323 (17)	0·0185 (30)
C(31)	0·0212 (22)	−0·0635 (23)	0·1383 (31)

The final atomic coordinates and their estimated standard deviations are listed in Table 1. Table 2 gives the atomic vibration parameters and their e.s.d.'s. The observed and calculated structure factors are listed in Table 3.

Discussion

The analysis shows the molecule to be a centrosymmetric dimer, with the p-bromophenyl groups in *trans* positions. Fig. 1 shows a projection down the c axis, with the numbering of the reference atoms indicated. Fig. 2 shows the central ten atoms of the molecule,

Table 2. *Vibration tensor components and e.s.d.'s* (Å^2)

	U_{11}	U_{22}	U_{33}	$2U_{23}$	$2U_{31}$	$2U_{12}$
Al	0·034 (2)	0·034 (2)	0·006 (2)	0·007 (3)	0·027 (4)	0·008 (3)
N	0·021 (6)	0·043 (5)	0·021 (7)	0·008 (9)	0·014 (9)	0·016 (8)
Br	0·129 (2)	0·037 (1)	0·070 (1)	−0·002 (1)	0·058 (2)	0·029 (2)
C(1)	0·038 (8)	0·043 (6)	0·002 (7)	−0·010 (10)	0·023 (12)	−0·021 (11)
C(2)	0·016 (7)	0·039 (6)	0·025 (8)	0·010 (11)	0·009 (12)	0·014 (10)
C(3)	0·057 (9)	0·039 (6)	0·026 (9)	0·029 (11)	0·061 (14)	0·033 (12)
C(4)	0·061 (10)	0·045 (7)	0·037 (10)	0·030 (13)	0·044 (16)	0·008 (13)
C(5)	0·044 (9)	0·045 (7)	0·065 (11)	−0·009 (14)	0·029 (16)	0·010 (13)
C(6)	0·075 (11)	0·047 (7)	0·028 (10)	0·025 (13)	0·041 (16)	0·038 (14)
C(7)	0·067 (10)	0·051 (7)	0·010 (8)	−0·015 (12)	0·023 (14)	0·026 (13)
C(8)	0·038 (8)	0·044 (6)	0·007 (8)	0·040 (11)	0·006 (12)	0·006 (11)
C(9)	0·029 (8)	0·060 (8)	0·044 (10)	0·023 (14)	−0·001 (14)	−0·013 (13)
C(10)	0·046 (10)	0·059 (9)	0·107 (15)	0·039 (19)	−0·015 (20)	0·005 (15)
C(11)	0·057 (12)	0·067 (10)	0·097 (16)	0·024 (20)	−0·050 (21)	−0·014 (16)
C(12)	0·077 (12)	0·050 (8)	0·046 (11)	0·014 (14)	−0·086 (18)	−0·009 (15)
C(13)	0·064 (10)	0·045 (7)	0·013 (8)	0·008 (11)	0·002 (14)	0·029 (13)
C(14)	0·028 (7)	0·046 (6)	0·015 (8)	0·024 (11)	0·028 (12)	0·021 (11)
C(15)	0·020 (7)	0·055 (7)	0·036 (9)	0·036 (13)	0·010 (13)	0·000 (11)
C(16)	0·062 (11)	0·068 (9)	0·062 (12)	0·070 (17)	0·063 (18)	0·024 (16)
C(17)	0·035 (9)	0·074 (10)	0·088 (14)	0·092 (19)	0·067 (18)	0·031 (14)
C(18)	0·072 (11)	0·082 (10)	0·051 (11)	0·078 (17)	0·081 (18)	0·040 (17)
C(19)	0·058 (9)	0·065 (8)	0·010 (8)	0·053 (13)	0·034 (14)	0·023 (14)
C(20)	0·035 (8)	0·030 (5)	0·018 (8)	0·015 (10)	0·020 (12)	0·019 (10)
C(21)	0·057 (9)	0·046 (6)	−0·001 (7)	−0·008 (10)	0·015 (12)	0·016 (12)
C(22)	0·074 (11)	0·070 (9)	0·032 (10)	−0·002 (15)	0·062 (17)	0·036 (16)
C(23)	0·057 (10)	0·094 (11)	0·027 (10)	−0·004 (16)	0·025 (16)	0·049 (17)
C(24)	0·051 (9)	0·071 (9)	0·019 (9)	0·010 (13)	0·038 (14)	0·015 (14)
C(25)	0·034 (8)	0·075 (9)	0·018 (9)	0·018 (13)	0·021 (14)	0·028 (13)
C(26)	0·226 (28)	0·102 (15)	0·069 (16)	0·076 (25)	0·064 (33)	0·163 (34)
C(27)	0·193 (25)	0·061 (11)	0·123 (21)	0·079 (25)	0·005 (35)	0·006 (26)
C(28)	0·164 (24)	0·232 (29)	0·146 (25)	0·354 (49)	0·143 (39)	0·094 (40)
C(29)	0·285 (38)	0·196 (29)	0·093 (21)	0·116 (40)	0·190 (46)	0·240 (55)
C(30)	0·208 (29)	0·097 (16)	0·133 (23)	0·073 (32)	−0·136 (42)	−0·048 (34)
C(31)	0·081 (17)	0·267 (33)	0·177 (27)	0·387 (54)	0·032 (33)	0·056 (35)

Table 3. *Observed and calculated structure factors*

H	K	L	Fo	Fo	H	K	L	Fo	Fo	H	K	L	Fo	Fc	H	K	L	Fo	Fc
1	0	0	42.7	-53.2	-1	13	0	25.9	26.0	-4	11	1	21.9	-20.2	3	-11	1	8.5	-7.2
2	0	0	22.4	-28.2	2	13	0	19.7	18.2	-3	11	1	19.8	17.7	4	-11	1	8.7	-11.1
3	0	0	60.3	84.0	3	13	0	8.4	-7.7	-2	11	1	15.3	14.2	5	-11	1	8.9	12.9
4	0	0	14.7	-13.0	-7	14	0	12.8	10.0	-1	11	1	34.2	-33.1	-4	-12	1	8.7	10.3
5	0	0	22.4	-22.7	-5	14	0	8.4	-7.1	0	11	1	25.1	24.5	-3	-12	1	12.7	-14.7
7	0	0	8.3	7.1	-4	14	0	19.4	19.7	2	11	1	25.5	-23.2	-2	-12	1	9.0	-9.3
8	0	0	33.4	-33.0	-3	14	0	19.7	-20.1	3	11	1	15.5	14.2	-1	-12	1	25.4	24.8
-8	1	0	25.1	20.8	-1	14	0	21.6	20.1	-8	12	1	7.7	8.6	0	-12	1	17.8	-14.1
-7	1	0	20.0	-17.0	0	14	0	17.4	-17.6	-7	12	1	11.9	-13.1	2	-12	1	21.7	24.8
-6	1	0	40.0	39.4	-6	15	0	15.9	-17.3	-4	12	1	18.0	-17.4	4	-12	1	15.5	-17.7
-5	1	0	22.2	-21.6	-1	15	0	11.5	11.5	-3	12	1	25.5	22.3	5	-12	1	9.0	10.5
-4	1	0	28.6	-31.0	1	15	0	10.7	-8.3	-1	12	1	12.7	-11.7	-3	-13	1	8.6	-1.5
-3	1	0	72.2	91.4	2	15	0	14.0	16.1	0	12	1	12.7	13.4	-2	-13	1	8.9	-9.6
-2	1	0	38.7	-52.4	-4	16	0	9.7	10.6	-6	13	1	20.3	21.2	-1	-13	1	12.7	13.0
2	1	0	80.0	-88.4	-3	16	0	7.1	-9.4	-5	13	1	14.9	-14.4	1	-13	1	22.1	-18.6
3	1	0	36.4	35.4	-1	16	0	14.0	16.5	-3	13	1	8.9	7.9	2	-13	1	22.1	19.0
4	1	0	19.9	20.8	0	16	0	15.1	-16.5	-1	13	1	12.6	-12.0	1	-14	1	12.5	-12.5
5	1	0	34.5	-36.8	-11	0	1	7.4	9.4	0	13	1	8.8	7.9	4	-14	1	17.5	-16.6
6	1	0	28.2	30.5	-9	0	1	9.0	-7.8	2	13	1	28.9	-30.2	5	-14	1	8.5	11.1
8	1	0	9.0	7.5	-8	0	1	37.1	36.5	-4	14	1	14.3	-13.8	-2	-15	1	10.5	-11.5
9	1	0	9.1	9.6	-7	0	1	22.8	-21.6	-3	14	1	20.5	22.0	-1	-15	1	17.6	18.9
-8	2	0	26.6	-22.2	-6	0	1	20.3	-16.1	-1	14	1	18.7	-18.7	1	-15	1	16.6	-16.7
-7	2	0	8.1	5.7	-5	0	1	46.7	46.8	0	14	1	23.2	23.5	2	-15	1	18.7	18.0
-6	2	0	14.6	9.1	-4	0	1	9.4	-9.5	-6	15	1	12.9	14.4	-8	0	2	31.3	-30.8
-3	2	0	33.8	36.4	-3	0	1	74.3	-83.0	-3	15	1	10.6	11.5	-7	0	2	26.4	24.6
-2	2	0	21.3	-24.8	-2	0	1	81.0	113.2	0	15	1	10.2	9.9	-6	0	2	12.9	8.9
-1	2	0	13.5	-12.7	1	0	1	25.2	27.8	2	15	1	10.7	-13.1	-5	0	2	52.7	-52.1
0	2	0	41.3	47.2	2	0	1	47.4	51.6	-3	16	1	10.9	13.2	-4	0	2	33.7	34.8
1	2	0	40.0	41.1	3	0	1	72.6	-82.3	-1	16	1	10.7	-11.5	-3	0	2	23.4	20.4
2	2	0	12.4	-12.8	4	0	1	55.6	64.5	0	16	1	11.7	13.8	-2	0	2	31.5	-36.5
3	2	0	20.1	25.2	-6	1	1	24.7	-19.2	-8	-1	1	15.3	10.3	1	0	2	108.3	-94.3
4	2	0	17.0	-15.5	-5	1	1	14.0	11.2	-7	-1	1	14.1	11.9	2	0	2	42.0	36.5
5	2	0	6.9	4.2	-4	1	1	40.0	32.9	-6	-1	1	30.2	-29.8	3	0	2	55.0	55.7
7	2	0	19.2	-10.8	-3	1	1	26.9	-33.9	-5	-1	1	77.9	76.9	4	0	2	52.3	-52.1
-8	3	0	8.9	-4.3	-2	1	1	20.2	-20.9	-4	-1	1	26.0	-22.9	5	0	2	17.4	19.6
-7	3	0	11.6	10.0	-1	1	1	17.3	-14.8	-3	-1	1	18.0	-23.2	6	0	2	11.3	-10.5
-5	3	0	55.3	-50.2	1	1	1	71.3	72.9	-2	-1	1	122.4	133.6	-8	1	2	18.0	16.4
-4	3	0	5.7	1.4	2	1	1	5.9	-8.1	-1	-1	1	39.1	-41.4	-6	1	2	24.7	18.1
-3	3	0	5.0	7.7	4	1	1	11.8	10.1	1	-1	1	25.9	36.3	-5	1	2	11.3	8.8
-2	3	0	78.0	-74.5	5	1	1	13.5	14.7	2	-1	1	33.7	-38.9	-4	1	2	38.0	38.0
-1	3	0	78.5	-73.8	6	1	1	21.6	-18.8	3	-1	1	36.5	-39.9	-3	1	2	20.9	23.8
0	3	0	47.7	55.7	-9	2	1	9.0	-7.1	4	-1	1	9.6	-7.7	-2	1	2	37.6	-37.4
1	3	0	37.9	-42.7	-6	2	1	12.4	-9.0	-7	-2	1	11.8	-7.9	-1	1	2	93.7	90.5
2	3	0	6.9	-5.6	-5	2	1	15.5	14.3	-6	-2	1	26.0	26.7	0	1	2	22.9	-17.1
3	3	0	41.3	45.9	-4	2	1	25.8	-26.6	-5	-2	1	11.5	-12.3	1	1	2	63.5	-61.1
5	3	0	14.4	-16.3	-3	2	1	9.5	-12.2	-4	-2	1	12.9	12.8	2	1	2	60.4	56.6
6	3	0	22.7	27.2	-2	2	1	19.3	20.4	-3	-2	1	17.0	-19.7	3	1	2	39.2	-30.3
7	3	0	27.7	21.5	-1	2	1	83.4	70.9	-2	-2	1	28.8	30.3	4	1	2	30.2	-29.5
-7	4	0	8.3	-4.7	0	2	1	28.9	22.4	-1	-2	1	82.6	89.8	5	1	2	7.3	6.3
-6	4	0	10.6	8.3	1	2	1	50.5	57.0	0	-2	1	48.4	-57.2	6	1	2	14.2	15.4
-5	4	0	22.2	-24.6	2	2	1	11.3	7.1	1	-2	1	55.0	61.9	-9	2	2	13.2	13.4
-4	4	0	16.9	19.2	3	2	1	23.4	-26.1	2	-2	1	87.5	-113.9	-7	2	2	11.8	10.6
-3	4	0	15.0	14.1	4	2	1	60.3	66.4	3	-2	1	14.9	9.2	-6	2	2	13.0	-9.5
-2	4	0	55.9	-59.6	5	2	1	19.9	-20.2	4	-2	1	15.7	14.5	-5	2	2	26.6	-21.3
-1	4	0	58.4	55.8	6	2	1	11.1	-10.7	5	-2	1	11.1	-8.3	-4	2	2	30.3	32.8
0	4	0	66.6	67.7	-8	3	1	8.7	6.6	6	-2	1	17.9	-14.0	-3	2	2	5.1	-4.5
1	4	0	32.5	-32.9	-7	3	1	18.0	-15.8	-7	-3	1	14.7	-12.2	-2	2	2	45.7	-44.9
2	4	0	27.9	-22.6	-6	3	1	7.3	-0.6	-6	-3	1	33.8	-37.0	-1	2	2	6.9	8.3
3	4	0	29.6	33.8	-5	3	1	24.2	23.5	-5	-3	1	31.7	31.0	1	2	2	44.8	-38.7
4	4	0	33.2	-33.1	-4	3	1	8.1	-9.1	-3	-3	1	28.9	-29.2	2	2	2	31.0	32.5
6	4	0	16.7	20.3	-3	3	1	13.3	9.7	-2	-3	1	20.2	23.5	3	2	2	44.4	44.0
7	4	0	28.3	-26.3	-2	3	1	113.6	101.4	-1	-3	1	9.5	10.6	4	2	2	13.5	-15.3
-8	5	0	20.1	-16.3	-1	3	1	23.7	-29.0	0	-3	1	19.5	-24.3	5	2	2	10.8	10.5
-7	5	0	14.6	10.9	0	3	1	59.0	-51.6	2	-3	1	83.9	91.3	6	2	2	18.9	20.5
-6	5	0	10.9	-9.2	1	3	1	52.5	45.0	3	-3	1	76.0	-87.5	7	2	2	15.8	-16.9
-5	5	0	24.2	-24.3	2	3	1	40.5	-36.5	4	-3	1	40.0	40.0	-9	3	2	9.3	-7.5
-4	5	0	6.3	-5.9	3	3	1	13.0	-11.0	6	-3	1	25.4	-22.1	-8	3	2	9.1	-9.7
-3	5	0	22.2	23.5	-5	4	1	22.2	22.6	-8	-4	1	18.0	15.1	-7	3	2	28.0	23.5
-2	5	0	15.1	-1.9	-4	4	1	21.6	-26.9	-7	-4	1	8.7	8.6	-6	3	2	21.7	-18.8
-1	5	0	10.2	7.9	-3	4	1	15.3	11.3	-6	-4	1	11.4	-10.7	-4	3	2	33.4	36.3
0	5	0	49.1	46.5	-2	4	1	47.1	48.4	-4	-4	1	6.5	5.5	-2	3	2	72.2	-56.5
1	5	0	60.3	-65.9	-1	4	1	95.5	-90.6	-3	-4	1	55.7	-58.7	-1	3	2	37.5	30.9
2	5	0	32.0	25.9	0	4	1	21.5	-20.9	-1	-4	1	25.8	27.1	0	3	2	16.4	-15.1
3	5	0	22.7	18.7	1	4	1	21.1	20.4	0	-4	1	94.8	-94.6	1	3	2	45.9	-42.3
4	5	0	17.7	-18.2	2	4	1	47.7	-42.9	1	-4	1	76.0	-71.9	2	3	2	12.7	12.5
5	5	0	13.8	11.8	4	4	1	29.6	27.3	3	-4	1	23.1	-25.9	3	3	2	18.1	15.2
6	5	0	8.7	-11.7	6	4	1	14.6	-13.4	5	-4	1	24.8	23.7	4	3	2	24.9	-25.2
-9	6	0	9.1	-9.4	7	4	1	12.6	9.2	6	-4	1	12.9	-12.2	5	3	2	11.3	13.7
-7	6	0	14.9	10.0	-8	5	1	15.4	11.2	7	-4	1	11.6	10.2	-9	4	2	13.2	-12.4
-6	6	0	22.5	20.7	-7	5	1	26.4	-22.5	-4	-5	1	15.4	15.9	-8	4	2	9.1	9.1
-5	6	0	24.2	-26.1	-6	5	1	10.9	10.0	-3	-5	1	27.0	-30.1	-5	4	2	23.6	-24.6
-4	6	0	30.0	32.5	-4	5	1	29.2	-29.6	-1	-5	1	26.5	29.7	-4	4	2	28.8	30.1
-3	6	0	41.7	42.1	-3	5	1	13.1	7.8	0	-5	1	38.3	-44.6	-3	4	2	34.8	-34.5
-2	6	0	86.5	-79.3	-2	5	1	7.8	11.2	1	-5	1	30.9	29.7	-2	4	2	17.3	-14.4
-1	6	0	59.7	52.2	-1	5	1	19.3	-20.8	2	-5	1	12.4	12.5	-1	4	2	75.5	66.4
0	6	0	10.1	11.0	0	5	1	19.6	17.7	3	-5	1	21.5	-21.0	0	4	2	25.9	-26.0
1	6	0	57.7	-56.4	1	5	1	18.1	19.9	4	-5	1	21.3	-23.4	1	4	2	25.6	-25.4
4	6	0	26.8	-25.0	2	5	1	12.4	-14.1	-8	-6	1	12.5	-12.1	2	4	2	59.3	59.0
5	6	0	11.9	-14.5	3	5	1	21.4	-18.2	-7	-6	1	20.1	20.4	4	4	2	7.6	-7.8
6	6	0	17.9	9.3	4	5	1	29.8	29.8	-6	-6	1	24.5	-21.5	5	4	2	8.4	9.8
-9	7	0	12.8	10.6	5	5	1	25.7	-25.2	-5	-6	1	27.9	31.0	-8	5	2	13.0	-9.7
-8	7	0	15.8	-12.8	-10	6	1	11.9	-11.6	-4	-6	1	7.4	7.2	-7	5	2	29.1	23.8
-7	7	0	24.9	20.5	-9	6	1	22.0	19.6	-3	-6	1	36.8	-36.2	-6	5	2	23.0	-20.0
-5	7	0	39.9	-36.2	-8	6	1	9.0	-4.4	-2	-6	1	19.5	19.8	-4	5	2	48.6	47.4
-4	7	0	22.6	19.4	-7	6	1	12.1	-7.9	-1	-6	1	36.6	30.5	-3	5	2	20.2	-18.1
-3	7	0	9.5	-10.5	-5	6	1	25.5	26.6	0	-6	1	30.9	-32.0	-2	5	2	51.4	44.5
-2	7	0	60.0	-55.7	-4	6	1	57.7	-56.8	1	-6	1	36.4	-32.1	-1	5	2	30.9	29.9
-1	7	0	20.1	18.2	-3	6	1	15.6	-13.1	2	-6	1	44.5	45.2	0	5	2	29.7	-32.6
0	7	0	47.8	46.7	-2	6	1	81.5	70.2	3	-6	1	42.7	-43.3	1	5	2	29.9	-28.1
1	7	0	37.9	-38.3	-1	6	1	50.6	-46.1	5	-6	1	20.2	23.3	2	5	2	25.6	23.7
2	7	0	7.1	-1.8	0	6	1	12.1	-9.1	6	-6	1	24.7	-25.0	3	5	2	23.6	-18.6
3	7	0	48.9	48.0	1	6	1	51.9	45.7	-7	-7	1	9.0	-13.7	4	5	2	19.9	-21.1
4	7	0	31.8	-33.1	2	6	1	57.4	-53.1	-6	-7	1	15.4	-18.2	5	5	2	15.2	14.9
5	7	0	12.4	8.8	3	6	1	10.4	8.6	-5	-7	1	12.0	-12.2	-10	6	2	20.9	20.2
6	7	0	18.2	20.7	4	6	1	15.9	15.2	-4	-7	1	45.9	45.1	-9	6	2	18.4	-16.4
-9	8	0	8.9	-8.1	-9	7	1	12.5	-13.9	-3	-7	1	61.7	-56.5	-7	6	2	22.0	20.7
-7	8	0	9.0	-7.2	-8	7	1	18.0	13.7	-2	-7	1	11.7	10.2	-6	6	2	28.0	-24.5
-6	8	0	8.6	7.3	-7	7	1	30.3	-26.7	-1	-7	1	69.7	73.7	-5	6	2	11.1	13.7
-5	8	0	14.0	-14.6	-5	7	1	27.9	25.6	0	-7	1	70.8	-66.8	-4	6	2	36.7	29.2
-3	8	0	20.6	17.5	-4	7	1	51.4	-42.9	1	-7	1	43.5	38.2	-2	6	2	60.4	-59.9
-2	8	0	24.5	-22.2	-3	7	1	37.7	33.6	2	-7	1	23.9	25.9	-1	6	2	28.8	48.4
-1	8	0	22.1	25.0	-2	7	1	56.5	48.4	3	-7	1	28.2	-28.2	0	6	2	34.9	-31.8
0	8	0	27.5	25.8	-1	7	1	9.3	-7.3	4	-7	1	12.0	-11.0	1	6	2	32.9	-33.0
1	8	0	31.2	-31.2	1	7	1	38.8	37.3	5	-7	1	23.7	23.8	2	6	2	35.0	37.3
2	8	0	18.9	20.7	2	7	1	20.8	-16.1	7	-7	1	12.2	-12.9	3	6	2	19.6	-18.4
3	8	0	11.6	-9.2	3	7	1	13.6	-11.2	8	-7	1	12.7	12.9	-7	7	2	9.2	8.1
-8	9	0	18.2	-17.4	4	7	1	29.0	27.1	-5	-8	1	8.8	7.8	-5	7	2	23.4	-19.8
-7	9	0	15.8	13.9	5	7	1	25.0	-22.2	-4	-8	1	14.4	-13.6	-4	7	2	40.7	38.3
-5	9	0	24.0	-20.9	-10	8	1	7.9	-8.0	-3	-8	1	11.1	-10.1	-3	7	2	53.5	-48.4
-4	9	0	28.2	25.4	-9	8	1	8.7	6.8	-1	-8	1	24.1	24.7	-2	7	2	7.3	7.5
-3	9	0	15.7	-13.5	-7	8	1	8.9	-7.1	0	-8	1	9.5	-8.2	-1	7	2	46.4	41.8
-2	9	0	29.7	-25.2	-6	8	1	8.6	8.0	1	-8	1	13.3	-13.3	0	7	2	40.4	-36.0
-1	9	0	21.6	20.8	-4	8	1	11.0	8.9	2	-8	1	47.2	46.7	2	7	2	19.7	19.9
0	9	0	10.9	9.8	-3	8	1	7.4	-3.8	3	-8	1	47.0	-45.2	4	7	2	18.0	-18.2
1	9	0	17.8	-17.2	-2	8	1	20.5	18.7	4	-8	1	7.4	6.9	5	7	2	13.1	13.3
2	9	0	11.7	12.0	-1	8	1	48.4	-45.3	5	-8	1	13.6	15.8	-6	8	2	25.6	-20.0
3	9	0	27.4	25.7	0	8	1	12.7	10.6	6	-8	1	11.9	-13.4	-5	8	2	17.4	15.0
4	9	0	22.1	-19.3	1	8	1	21.5	18.4	-4	-9	1	19.5	17.9	-3	8	2	25.5	-21.9
-7	10	0	18.3	12.9	2	8	1	43.5	-38.4	-3	-9	1	26.4	-22.8	-1	8	2	37.0	34.3
-6	10	0	9.1	-8.4	3	8	1	20.5	19.1	-1	-9	1	13.1	12.6	0	8	2	22.7	-23.5
-4	10	0	19.2	17.2	5	8	1	20.1	-17.9	0	-9	1	28.5	-25.8	1	8	2	20.3	-19.1
-2	10	0	26.1	-22.9	-5	9	1	24.2	22.3	1	-9	1	10.3	-11.2	2	8	2	50.2	52.6
-1	10	0	40.4	39.3	-4	9	1	42.8	-36.8	2	-9	1	12.7	11.8	3	8	2	31.1	-33.9
1	10	0	36.2	-32.4	-3	9	1	11.3	12.1	3	-9	1	10.7	-9.2	5	8	2	22.8	25.8
2	10	0	24.8	21.6	-2	9	1	13.6	10.8	4	-9	1	19.3	-20.4	-6	9	2	9.2	-7.6
4	10	0	18.3	-17.6	-1	9	1	27.2	-26.4	5	-9	1	23.4	23.6	-5	9	2	12.8	-10.6
5	10	0	12.8	-4.2	0	9	1	15.9	15.0	7	-9	1	9.0	-10.1	-4	9	2	39.4	33.6
-5	11	0	12.9	-13.4	1	9	1	11.5	8.7	8	-9	1	18.0	18.4	-3	9	2	19.2	-15.8
-4	11	0	25.3	24.5	2	9	1	14.7	-14.8	-7	-10	1	7.9	-4.1	-1	9	2	35.0	32.9
-3	11	0	15.3	-15.6	3	9	1	12.4	-13.3	-4	-10	1	18.0	18.4	0	9	2	29.8	-27.6
-2	11	0	33.9	-30.0	4	9	1	20.1	20.8	-3	-10	1	8.8	-9.0	2	9	2	15.7	14.2
-1	11	0	32.7	27.9	-7	10	1	22.0	-17.9	-2	-10	1	8.5	-8.0	-6	10	2	22.8	-22.1
0	11	0	12.5	-11.8	-6	10	1	12.7	12.1	-1	-10	1	44.8	43.1	-5	10	2	22.7	23.0
1	11	0	20.0	-20.9	-5	10	1	15.3	-14.5	0	-10	1	22.6	-16.8	-4	10	2	25.9	22.0
2	11	0	15.8	13.6	-4	10	1	27.4	-22.5	1	-10	1	13.7	-13.7	-3	10	2	42.4	-35.3
-7	12	0	17.5	16.0	-3	10	1	26.8	22.8	2	-10	1	25.1	23.7	-2	10	2	12.7	12.5
-5	12	0	15.9	-14.0	-2	10	1	8.4	8.0	3	-10	1	16.2	-15.3	0	10	2	20.3	-14.8
-4	12	0	20.5	18.7	-1	10	1	29.1	-24.2	5	-10	1	14.9	15.6	2	10	2	9.3	8.5
-2	12	0	9.1	-9.1	1	10	1	27.4	24.5	6	-10	1	12.6	-12.1	3	10	2	9.3	-8.0
-1	12	0	15.7	12.5	2	10	1	25.0	-21.6	-4	-11	1	15.6	16.9	-9	11	2	7.3	-7.9
0	12	0	9.1	7.4	3	10	1	15.6	15.2	-3	-11	1	9.0	-12.3	-8	11	2	8.2	8.1
1	12	0	22.4	-21.8	4	10	1	12.7	9.4	-2	-11	1	8.9	-10.5	-7	11	2	12.5	11.6
2	12	0	9.1	9.9	-8	11	1	8.3	-6.9	-1	-11	1	24.5	22.9	-6	11	2	13.0	-13.6
-4	13	0	9.1	5.4	-6	11	1	12.7	10.8	1	-11	1	26.7	-25.3	-5	11	2	16.1	18.7
-2	13	0	18.3	-18.5	-5	11	1	9.0	9.1	2	-11	1	20.7	19.0	-4	11	2	9.3	-8.7

Table 3 (*cont.*)

H	K	L	Fo	Fc
-3	11	2	13.1	-11.6
-1	11	2	20.8	15.3
0	11	2	34.8	-31.6
2	11	2	16.0	17.2
3	11	2	22.1	-22.2
4	11	2	8.5	9.2
-7	12	2	8.3	-7.9
-5	12	2	9.1	-8.6
-4	12	2	16.0	15.2
-3	12	2	22.7	-23.2
-2	12	2	13.1	11.9
-1	12	2	9.3	10.8
0	12	2	22.6	-20.4
1	12	2	22.3	18.6
3	12	2	8.4	-7.1
-6	13	2	14.1	-14.8
-5	13	2	14.8	18.2
-3	13	2	15.4	-16.6
-2	13	2	15.5	17.6
0	13	2	17.5	-19.7
2	13	2	11.4	11.8
3	13	2	10.4	-11.3
-5	14	2	10.9	13.4
-3	14	2	14.1	-14.9
-2	14	2	11.6	12.0
-1	14	2	8.1	7.1
0	14	2	17.6	-17.7
1	14	2	19.8	20.8
3	14	2	8.4	-11.5
-3	15	2	10.0	-13.2
-2	15	2	12.3	16.5
0	15	2	9.4	-10.3
-8	-1	2	22.3	-19.1
-7	-1	2	8.4	6.8
-5	-1	2	31.1	-34.5
-4	-1	2	36.4	41.1
-3	-1	2	27.7	30.9
-2	-1	2	95.3	-108.2
1	-1	2	59.3	-70.1
2	-1	2	26.2	32.2
3	-1	2	7.2	9.1
5	-1	2	12.0	-10.9
-9	-2	2	9.3	9.7
-8	-2	2	9.2	10.6
-7	-2	2	24.2	23.2
-6	-2	2	26.8	-28.2
-4	-2	2	22.8	23.3
-3	-2	2	48.0	-44.4
-2	-2	2	12.8	-13.9
-1	-2	2	5.3	-2.4
0	-2	2	67.8	-73.7
1	-2	2	88.1	-104.4
2	-2	2	34.7	-35.5
3	-2	2	43.8	46.5
4	-2	2	53.4	-58.8
5	-2	2	19.4	22.9
-6	-3	2	26.4	23.5
-5	-3	2	28.3	-31.6
-4	-3	2	33.9	35.3
-2	-3	2	55.5	-49.5
-1	-3	2	61.5	62.1
0	-3	2	32.4	32.4
1	-3	2	64.8	-63.3
2	-3	2	19.3	17.6
3	-3	2	17.0	20.7
4	-3	2	23.2	-26.5
5	-3	2	26.6	-28.6
6	-3	2	31.1	32.4
7	-3	2	31.0	-24.5
-6	-4	2	8.2	10.2
-4	-4	2	13.1	-11.2
-3	-4	2	53.3	53.4
-2	-4	2	46.5	-48.0
-1	-4	2	18.7	-18.2
0	-4	2	60.2	-38.5
1	-4	2	129.4	-127.9
2	-4	2	42.2	40.0
3	-4	2	7.6	9.6
4	-4	2	17.4	-20.0
5	-4	2	9.9	-10.3
6	-4	2	13.6	10.9
-8	-5	2	16.1	-14.4
-7	-5	2	18.3	-18.7
-5	-5	2	17.4	-19.7
-3	-5	2	6.2	-4.5
-2	-5	2	5.6	-6.0
-1	-5	2	11.3	8.6
0	-5	2	65.9	60.1
1	-5	2	19.9	-20.5
2	-5	2	17.9	-18.3
3	-5	2	54.3	57.5
4	-5	2	33.3	-36.7
5	-5	2	33.7	39.8
6	-5	2	11.3	-10.4
-5	-6	2	16.4	-17.5
-4	-6	2	10.6	-9.1
-3	-6	2	21.4	22.8
-2	-6	2	44.1	-40.6
-1	-6	2	9.9	-12.7
1	-6	2	28.3	-26.1
2	-6	2	11.4	-12.0
3	-6	2	22.2	25.2
4	-6	2	6.7	-7.6
5	-6	2	26.8	-33.4
6	-6	2	32.7	35.1
7	-6	2	8.8	-9.7
-8	-7	2	17.9	-19.1
-6	-7	2	15.8	15.2
-5	-7	2	8.6	-9.9
-4	-7	2	16.0	-15.1
-3	-7	2	32.0	29.8
-2	-7	2	23.5	-24.1
-1	-7	2	34.3	-29.9
0	-7	2	63.6	60.9
1	-7	2	25.8	-26.7
2	-7	2	6.3	-4.9
3	-7	2	26.5	28.8
6	-7	2	8.4	11.6
-6	-8	2	22.8	25.1
-5	-8	2	31.1	-29.9
-4	-8	2	24.0	23.6
-3	-8	2	28.5	25.9
-2	-8	2	7.4	-8.6
-1	-8	2	12.2	11.4
0	-8	2	11.7	9.6
1	-8	2	13.5	-16.1
2	-8	2	24.7	-24.4
3	-8	2	39.9	42.2
4	-8	2	7.6	-8.8
5	-8	2	16.3	-17.0
6	-8	2	8.7	12.2
-5	-9	2	16.0	14.0
-4	-9	2	29.5	-27.8
-3	-9	2	30.5	28.7
-2	-9	2	26.6	-22.2
0	-9	2	49.9	46.6
1	-9	2	33.8	-33.0
2	-9	2	12.9	-13.5
3	-9	2	7.7	9.4
4	-9	2	14.0	15.1
6	-9	2	9.0	11.0
-6	-10	2	9.1	12.0
-5	-10	2	9.3	-13.3
-3	-10	2	12.6	10.4
-2	-10	2	8.6	5.7
-1	-10	2	26.2	-24.7
0	-10	2	29.2	29.4
2	-10	2	37.0	-34.1
3	-10	2	42.9	38.2
4	-10	2	24.2	-25.3
5	-10	2	12.6	-14.6
6	-10	2	13.0	16.0
-4	-11	2	9.3	-11.7
-3	-11	2	13.1	11.4
-2	-11	2	9.0	-8.3
-1	-11	2	17.7	-16.6
0	-11	2	8.7	7.6
2	-11	2	8.6	-6.8
3	-11	2	17.5	17.7
6	-11	2	9.3	11.7
-4	-12	2	12.9	-10.8
-3	-12	2	22.8	22.2
-1	-12	2	18.4	-16.9
0	-12	2	20.4	19.1
2	-12	2	20.3	-22.2
4	-12	2	13.1	11.4
-1	-13	2	9.3	-9.7
0	-13	2	16.1	15.3
1	-13	2	9.3	9.6
2	-13	2	22.8	-19.6
3	-13	2	18.6	17.7
-4	-14	2	10.9	-10.8
-3	-14	2	8.4	9.2
-1	-14	2	12.8	-12.4
0	-14	2	9.2	9.0
2	-14	2	9.2	-11.7
-2	-15	2	8.0	10.0
-1	-15	2	14.6	-15.5
1	-15	2	12.5	12.0
2	-15	2	17.7	-15.8
3	-15	2	12.4	11.3
-8	0	3	27.1	22.5
-7	0	3	29.5	-24.1
-6	0	3	8.0	6.2
-5	0	3	31.4	26.4
-4	0	3	42.7	-41.7
-3	0	3	24.3	24.7
-2	0	3	4.1	-1.5
-1	0	3	20.9	-23.0
0	0	3	31.7	24.1
1	0	3	18.5	16.5
2	0	3	33.3	-34.2
3	0	3	16.8	-13.8
4	0	3	12.0	11.6
5	0	3	22.3	-23.8
-9	1	3	9.8	9.2
-8	1	3	9.6	-11.6
-7	1	3	8.9	-5.4
-6	1	3	19.6	16.7
-5	1	3	22.4	-19.7
-4	1	3	23.8	-19.6
-3	1	3	5.3	-6.7
-2	1	3	37.9	28.3
-1	1	3	143.7	-109.3
0	1	3	33.7	30.0
1	1	3	43.5	40.9
2	1	3	56.3	-55.4
3	1	3	37.9	33.9
4	1	3	36.2	37.7
5	1	3	23.1	-22.0
-9	2	3	13.9	-12.0
-7	2	3	12.7	-9.4
-5	2	3	34.7	29.2
-4	2	3	36.2	-36.8
-3	2	3	39.8	39.5
-2	2	3	19.4	20.3
-1	2	3	28.0	-28.3
0	2	3	22.4	21.7
1	2	3	43.3	42.9
2	2	3	5.9	5.0
3	2	3	6.8	-6.8
4	2	3	13.2	12.5
5	2	3	17.0	-20.3
-9	3	3	13.8	10.9
-8	3	3	13.6	10.9
-7	3	3	25.7	-15.7
-6	3	3	30.0	25.7
-4	3	3	24.3	-23.7
-3	3	3	51.6	45.6
-2	3	3	29.1	-23.9
-1	3	3	50.0	-43.2
1	3	3	22.9	20.1
2	3	3	33.3	-34.8
3	3	3	14.5	13.7
6	3	3	13.5	15.2
-9	4	3	19.5	17.7
-8	4	3	16.8	-18.8
-7	4	3	9.2	7.5
-6	4	3	29.7	29.4
-5	4	3	22.2	-20.6
-4	4	3	10.1	7.7
-3	4	3	14.8	15.2
-2	4	3	24.9	20.0
-1	4	3	51.7	-52.9
0	4	3	44.0	44.3
2	4	3	37.2	-36.7
3	4	3	27.1	24.4
-10	5	3	15.5	14.7
-7	5	3	13.3	-9.5
-6	5	3	8.9	6.0
-4	5	3	45.8	-44.4
-3	5	3	56.9	50.8
-2	5	3	41.3	-38.2
-1	5	3	40.8	-39.3
0	5	3	27.7	27.1
1	5	3	17.8	-14.5
3	5	3	11.9	11.4
4	5	3	9.0	10.3
5	5	3	19.1	-21.4
6	5	3	9.8	13.4
-10	6	3	17.4	-19.7
-9	6	3	16.5	14.5
-8	6	3	9.8	-9.5
-7	6	3	13.6	-10.7
-6	6	3	35.5	35.9
-5	6	3	12.2	-12.3
-4	6	3	18.2	-16.7
-3	6	3	19.0	15.8
-2	6	3	18.5	14.3
-1	6	3	24.9	-23.7
0	6	3	33.3	30.0
1	6	3	8.0	6.6
2	6	3	38.5	-36.4
3	6	3	28.2	25.3
4	6	3	16.3	-15.1
-5	7	3	12.8	-11.7
-4	7	3	23.0	-21.3
-3	7	3	62.6	60.5
-2	7	3	29.5	-29.9
-1	7	3	25.9	-25.7
0	7	3	67.1	59.4
1	7	3	25.8	-20.9
3	7	3	21.0	20.8
-6	8	3	37.6	36.4
-5	8	3	9.5	-10.2
-3	8	3	34.6	32.4
-2	8	3	30.5	-28.6
-1	8	3	12.5	-12.4
0	8	3	15.5	15.4
2	8	3	49.2	-44.3
3	8	3	16.8	16.6
4	8	3	9.8	11.3
5	8	3	21.4	-23.8
6	8	3	8.9	12.0
-9	9	3	8.5	8.2
-8	9	3	9.3	-8.1
-5	9	3	9.7	-12.4
-2	9	3	13.2	11.4
-1	9	3	36.3	-31.3
0	9	3	23.2	24.2
3	9	3	13.9	13.2
-6	10	3	9.7	9.8
-5	10	3	9.8	-10.7
-4	10	3	9.8	-10.0
-3	10	3	27.5	25.5
-2	10	3	32.2	-28.6
0	10	3	16.9	17.3
1	10	3	24.0	-23.3
-5	11	3	16.7	-19.6
-4	11	3	9.7	10.1
-3	11	3	24.0	23.9
-2	11	3	27.7	-26.0
0	11	3	13.8	16.5
1	11	3	9.6	-10.3
3	11	3	15.5	18.6
4	11	3	8.2	-7.9
-2	12	3	19.0	-17.4
0	12	3	20.9	19.9
1	12	3	24.0	-22.3
-6	13	3	7.8	11.8
-5	13	3	16.7	-20.5
-3	13	3	8.8	12.8
-2	13	3	19.8	-19.4
-5	14	3	7.2	-8.9
-2	14	3	11.0	-13.1
0	14	3	14.6	16.9
1	14	3	15.1	-17.6
-3	15	3	8.9	11.1
-2	15	3	10.9	-14.6
-10	-1	3	20.6	-21.3
-9	-1	3	19.6	18.8
-8	-1	3	9.6	8.1
-5	-1	3	44.7	45.7
-4	-1	3	26.4	-47.4
-3	-1	3	27.6	-23.6
-2	-1	3	33.3	47.6
-1	-1	3	52.9	-67.6
1	-1	3	35.2	33.3
2	-1	3	37.4	-35.6
3	-1	3	24.8	18.8
-7	-2	3	31.4	-26.8
-6	-2	3	31.7	28.3
-4	-2	3	19.7	-19.4
-3	-2	3	44.2	46.5
-2	-2	3	16.5	16.2
-1	-2	3	42.5	-39.6
0	-2	3	58.8	-54.6
1	-2	3	22.5	34.9
2	-2	3	14.3	-19.7
3	-2	3	15.7	-16.0
4	-2	3	6.6	6.7
5	-2	3	30.2	-30.2
-4	-3	3	43.6	-44.7
-3	-3	3	37.1	-36.8
-2	-3	3	82.5	87.2
-1	-3	3	60.3	-57.3
0	-3	3	45.6	-37.1
1	-3	3	12.4	13.9
2	-3	3	19.7	-25.5
3	-3	3	11.2	-10.3
4	-3	3	36.6	36.0
6	-3	3	26.8	-21.2
-8	-4	3	9.8	9.9
-7	-4	3	23.1	-19.5
-5	-4	3	17.4	15.7
-4	-4	3	31.5	-30.7
-2	-4	3	7.3	7.3
-1	-4	3	44.9	-43.9
0	-4	3	38.9	-34.4
1	-4	3	65.8	69.3
2	-4	3	24.4	-24.1
3	-4	3	25.3	-31.5
4	-4	3	32.7	37.4
5	-4	3	33.1	-31.5
-5	-5	3	20.0	22.3
-4	-5	3	25.3	-29.0
-2	-5	3	12.9	16.7
-1	-5	3	43.9	-40.9
0	-5	3	37.8	-33.0
1	-5	3	20.0	21.0
6	-5	3	12.2	-12.9
-6	-6	3	13.1	-11.9
-5	-6	3	14.9	17.3
-3	-6	3	12.2	-11.8
-2	-6	3	69.1	64.6
-1	-6	3	52.9	-49.6
1	-6	3	57.2	57.4
2	-6	3	32.8	27.9
3	-6	3	9.2	8.5
5	-6	3	13.9	16.0
6	-6	3	6.6	-7.8
-5	-7	3	12.7	13.7
-4	-7	3	14.4	-15.0
-3	-7	3	18.7	-17.6
-2	-7	3	28.1	29.8
-1	-7	3	25.5	24.1
0	-7	3	61.8	-62.7
1	-7	3	30.4	34.3
2	-7	3	25.5	-23.2
3	-7	3	30.6	-32.9
4	-7	3	39.6	50.1
5	-7	3	14.4	-16.8
6	-7	3	9.0	11.1
-6	-8	3	13.8	-15.7
-5	-8	3	21.0	20.9
-4	-8	3	8.8	-9.3
-3	-8	3	26.0	-24.7
-2	-8	3	42.2	40.5
-1	-8	3	23.0	-22.5
0	-8	3	7.1	6.6
1	-8	3	47.1	47.5
2	-8	3	26.9	27.5
3	-8	3	29.3	-28.0
5	-8	3	17.3	19.1
6	-8	3	24.5	-29.2
7	-8	3	19.4	20.1
-2	-9	3	18.7	16.5
-1	-9	3	8.0	7.6
0	-9	3	58.0	-54.4
1	-9	3	24.3	23.3
3	-9	3	16.2	-16.0
4	-9	3	12.1	11.6
-6	-10	3	19.2	-19.9
-5	-10	3	19.6	20.7
-4	-10	3	13.6	-12.4
-2	-10	3	25.3	26.1
0	-10	3	23.8	-23.6
1	-10	3	20.5	20.9
2	-10	3	23.9	21.4
3	-10	3	28.8	-29.7
4	-10	3	22.1	22.7
5	-10	3	13.3	12.1
6	-10	3	13.7	-16.4
7	-10	3	9.8	11.1
-3	-11	3	27.4	-27.6
-2	-11	3	34.1	33.1
-1	-11	3	9.2	-9.7
0	-11	3	20.2	-17.3
1	-11	3	22.0	21.1
2	-11	3	15.6	-14.9
4	-11	3	16.3	15.8
6	-11	3	9.8	-12.8
7	-11	3	9.7	8.9
-2	-12	3	9.7	-9.4
-1	-12	3	16.7	15.4
0	-12	3	26.9	-27.7
1	-12	3	9.5	8.3
2	-12	3	9.5	11.0
3	-12	3	9.6	-11.1
-2	-13	3	13.8	13.3
0	-13	3	9.8	-12.0
2	-13	3	23.9	21.9
3	-13	3	13.9	-12.1
5	-13	3	9.7	11.1
6	-13	3	9.5	-12.8
-3	-14	3	12.7	-12.7
0	-14	3	21.7	-18.9
-1	-15	3	12.8	13.8
2	-15	3	18.7	17.3
3	-15	3	13.1	-14.0
-10	0	4	9.2	-12.2
-8	0	4	9.7	-8.7
-7	0	4	13.0	12.2
-6	0	4	20.3	-18.2
-5	0	4	10.4	5.5
-4	0	4	47.5	50.8
-3	0	4	55.7	-65.6
-2	0	4	32.9	33.0
-1	0	4	15.9	20.0
0	0	4	66.7	-64.9
1	0	4	34.3	30.0
2	0	4	11.1	10.9
3	0	4	22.7	-22.2
4	0	4	21.3	-20.4
5	0	4	19.0	18.5
6	0	4	13.1	-12.8
-8	1	4	9.7	8.9
-7	1	4	15.9	12.0
-6	1	4	32.4	-29.2
-5	1	4	32.5	30.5
-4	1	4	25.3	29.0
-3	1	4	53.8	-61.1
-2	1	4	24.2	-20.3
-1	1	4	42.8	39.8
0	1	4	12.3	8.6
1	1	4	26.3	-18.0
2	1	4	70.5	70.9
3	1	4	32.7	-34.6
5	1	4	15.2	15.6
-10	2	4	9.1	11.7
-9	2	4	13.9	-9.5
-8	2	4	16.9	17.5
-5	2	4	13.3	-11.9
-3	2	4	8.6	-6.9
-2	2	4	21.5	-18.8
-1	2	4	55.1	48.0
0	2	4	38.5	-36.6
1	2	4	8.4	5.7
2	2	4	9.4	8.7
3	2	4	10.5	-10.2
-10	3	4	9.0	-8.9
-8	3	4	9.8	-11.7
-7	3	4	9.4	9.2
-6	3	4	27.6	-24.3
-5	3	4	8.0	7.3
-4	3	4	25.1	23.0
-3	3	4	46.9	-42.9
-2	3	4	17.5	16.5
-1	3	4	10.5	-2.9
0	3	4	35.7	-35.3
1	3	4	16.3	13.3
2	3	4	12.6	11.6
3	3	4	16.0	-16.7
5	3	4	18.8	16.2
6	3	4	9.8	-12.7
-9	4	4	13.7	-14.6
-8	4	4	19.7	17.0
-6	4	4	23.8	-22.4
-5	4	4	20.4	19.7
-4	4	4	7.7	-6.2
-3	4	4	26.0	-21.2
-2	4	4	24.8	23.7
-1	4	4	13.6	14.3
0	4	4	65.9	-36.2
1	4	4	23.2	21.8
2	4	4	30.5	25.7
3	4	4	27.0	-23.0
4	4	4	15.9	14.6
-5	5	4	17.5	16.2
-4	5	4	20.1	19.2
-3	5	4	46.8	-43.9
-2	5	4	29.2	28.0
0	5	4	36.0	-32.8
1	5	4	37.6	35.4
2	5	4	19.0	-17.6
3	5	4	22.2	-22.6
5	5	4	9.6	12.4
-9	6	4	9.3	-7.9
-8	6	4	9.6	9.6
-7	6	4	17.0	15.7
-6	6	4	23.4	-22.1
-5	6	4	25.9	27.0
-4	6	4	24.7	-23.0
-3	6	4	14.6	-13.5
-2	6	4	38.6	39.6
-1	6	4	16.3	-17.0
1	6	4	8.7	-10.5
2	6	4	22.2	22.5
3	6	4	19.0	-18.0
4	6	4	13.9	14.1
6	6	4	16.3	-18.6
-8	7	4	16.7	16.6
-7	7	4	24.2	-23.8
-5	7	4	21.2	21.4
-3	7	4	34.7	-31.7
-2	7	4	19.8	16.6
-1	7	4	25.0	22.3
0	7	4	60.3	-56.1
1	7	4	55.4	54.3
3	7	4	24.0	-27.2
4	7	4	13.9	12.7
-7	8	4	13.8	12.3
-6	8	4	19.7	-21.1
-5	8	4	13.8	14.2
-3	8	4	36.6	-33.7
-2	8	4	29.7	28.7
0	8	4	26.9	-24.3
1	8	4	9.7	8.7
2	8	4	13.9	12.2
3	8	4	9.9	-11.4
-3	9	4	9.8	-8.0
-2	9	4	9.7	12.1
-1	9	4	9.8	-7.9
0	9	4	9.8	8.1
1	9	4	13.9	14.1
4	9	4	9.1	9.8
-8	10	4	8.2	9.3
-7	10	4	9.0	-8.1
-5	10	4	13.7	18.9
-4	10	4	17.0	-16.7
-2	10	4	22.0	23.7
-1	10	4	17.1	-14.2
0	10	4	17.0	-16.1
1	10	4	13.7	15.9
2	10	4	13.4	-12.9
-5	11	4	20.7	21.3
-4	11	4	19.0	-23.9
-2	11	4	16.7	17.3
-1	11	4	19.2	-18.5
1	11	4	16.0	15.8
-2	12	4	15.6	15.8
0	12	4	12.3	-13.3
1	12	4	14.4	18.5
2	12	4	10.9	-11.6
-5	13	4	12.9	15.9
-4	13	4	7.8	-10.4
-2	13	4	16.1	18.6
-1	13	4	15.8	-17.5
1	13	4	7.0	9.1
-4	14	4	12.8	-16.3
-2	14	4	9.4	11.3
-10	-1	4	18.2	19.9
-9	-1	4	17.0	-17.8
-6	-1	4	18.6	-19.0
-5	-1	4	14.7	-12.5
-4	-1	4	12.6	-12.4
-2	-1	4	26.2	-27.9
-1	-1	4	71.0	68.9
0	-1	4	44.2	-44.8
1	-1	4	5.6	-3.4
2	-1	4	43.7	48.3
3	-1	4	24.1	-25.8
-7	-2	4	26.2	26.0
-6	-2	4	18.8	-18.1
-4	-2	4	22.2	25.8
-3	-2	4	48.0	-61.4
-2	-2	4	19.0	16.9
-1	-2	4	18.6	20.5
1	-2	4	26.0	-28.4
3	-2	4	14.8	-16.8

Table 3 (*cont.*)

H	K	L	Fo	Fc
4	-2	4	32.4	-32.0
5	-2	4	22.9	20.6
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2	-12	6	13.3	8.0
-8	0	7	16.5	-17.1
-7	0	7	25.5	23.3
-5	0	7	8.6	10.5
-4	0	7	7.8	10.6
-1	0	7	10.4	6.6
0	0	7	23.6	18.3
1	0	7	35.9	-33.9
2	0	7	7.9	9.7
4	0	7	22.9	-23.7
5	0	7	13.6	15.7
-8	1	7	9.5	10.6
-7	1	7	13.7	-14.4
-5	1	7	8.9	-8.7
-3	1	7	10.6	13.0
-2	1	7	26.4	-28.1
-1	1	7	21.9	16.7
2	1	7	26.7	21.8
-7	2	7	9.7	11.2
-5	2	7	12.9	-16.2
-4	2	7	27.2	26.3
-3	2	7	14.0	-10.2
-2	2	7	24.6	-24.4
-1	2	7	26.8	23.2
1	2	7	25.2	-23.6
-7	3	7	13.6	12.9
-6	3	7	23.6	-24.1
-4	3	7	18.0	20.5
-3	3	7	15.0	-16.8
-1	3	7	14.6	10.9
2	3	7	36.2	39.5
4	3	7	13.6	-11.2
-5	4	7	13.5	-15.1
-4	4	7	18.7	20.0
-2	4	7	22.1	-21.5
-1	4	7	35.0	35.6
0	4	7	20.5	-16.9
4	4	7	13.3	-12.4
-7	5	7	16.0	18.1
-6	5	7	21.4	-24.4
-4	5	7	13.6	11.8
0	5	7	13.5	14.4
1	5	7	23.6	-21.7
2	5	7	13.6	11.8
-4	6	7	16.7	15.6
-3	6	7	13.7	-15.7
-2	6	7	21.6	-18.3
-1	6	7	32.0	31.2
0	6	7	23.7	-22.8
2	6	7	16.4	16.1
3	6	7	9.0	-11.1
-4	7	7	16.5	18.6
-3	7	7	16.6	-19.0
-2	7	7	13.6	9.8
0	7	7	13.4	-12.5
-1	8	7	13.0	13.6
-4	9	7	11.8	17.1
-3	9	7	8.5	-11.2
-1	9	7	14.7	19.1
0	9	7	11.6	-12.1
-5	-1	7	24.0	-27.9
-4	-1	7	23.9	26.4
-3	-1	7	11.3	11.9
-2	-1	7	30.1	-25.1
-1	-1	7	27.0	23.1
0	-1	7	15.1	-12.7
1	-1	7	12.6	11.5
3	-1	7	14.4	13.9
5	-1	7	16.6	-18.9
-6	-2	7	18.4	16.6
-5	-2	7	18.9	-13.6
-1	-2	7	11.6	-10.5
0	-2	7	33.7	34.5
1	-2	7	33.8	-29.5
3	-2	7	11.3	9.1
-5	-3	7	24.0	-21.3
-4	-3	7	23.6	24.1
-2	-3	7	25.8	-39.6
1	-3	7	22.5	-25.0
3	-3	7	20.5	19.0
-5	-4	7	12.2	12.6
-4	-4	7	7.7	-6.5
-3	-4	7	33.1	38.5
-2	-4	7	30.7	-34.7
-1	-4	7	26.0	19.1
0	-4	7	14.1	10.7
1	-4	7	26.1	-32.2
2	-4	7	20.5	22.9
-5	-5	7	28.1	-31.4
-4	-5	7	13.9	15.4
-3	-5	7	9.9	11.2
-2	-5	7	18.5	16.3
-1	-5	7	40.9	-36.6
0	-5	7	21.8	17.0
3	-5	7	18.9	19.2
-2	-6	7	28.1	-21.0
-1	-6	7	32.8	25.3
-2	-7	7	41.8	-35.7
-1	-7	7	21.6	-16.3
0	-7	7	29.7	24.8
1	-7	7	26.7	-25.4
-4	-8	7	13.0	13.0
-3	-8	7	15.0	15.7
-1	-8	7	23.0	-22.2
2	-8	7	31.2	-31.4
3	-8	7	19.2	14.1
4	-8	7	13.0	-14.6
-4	-9	7	23.3	-23.5
-3	-9	7	25.9	25.2
1	-9	7	18.5	-17.1
4	-9	7	13.3	12.5
0	-10	7	34.3	30.0
1	-10	7	12.6	-16.0
2	-10	7	12.8	-8.8
3	-10	7	18.7	20.1
4	-10	7	9.6	-16.1
-4	-11	7	13.6	-13.4
-3	-11	7	13.7	9.8
-2	-11	7	16.6	-16.7
-4	-12	7	9.3	-8.6
-3	-12	7	13.5	12.2
-1	-12	7	23.6	-19.1

with their displacements from the weighted mean plane. There is no significant deviation from planarity. The bond lengths and their e.s.d.'s are given in Table 4, and the equations of the best planes through the central ten atoms and through the five benzene rings are given in Table 5. The principal bond angles are shown in Fig. 2.

The two independent Al–N bond lengths, 1·916 Å and 1·918 Å, are close to the values for four coordinated aluminum in aluminum nitride (mean = 1·893 Å) (Jeffrey, Parry & Mozzi, 1956) and in (PhAlNPh)₄ (mean = 1·914 Å) (McDonald & McDonald, 1963). The Al–N–Al angle of 97·1° is presumably increased as a result of the double bond. Both N–C–C angles are significantly greater than 120°, perhaps as a result of non-bonded

repulsions. The relevant non-bonded distances are N–C(2) = 2·43 Å, N–C(8) = 2·45 Å, C(2)–C(8) = 2·48 Å. The N–C(1) distance of 1·28 Å is that expected for a double bond, and the Al–C distances are in close agreement with those found for the terminal Al–C distances in triphenyl aluminum (Malone & McDonald, 1967).

The molecule of benzene is undergoing thermal vibrations of large amplitude. For a planar molecule with all atoms equidistant from the centre it is not possible to carry out a full analysis of the rigid body vibrations and librations (Cruickshank, 1956). In any case the accuracy of the U_{ij} scarcely justify such a treatment in this case. It is clear, however, that the molecule executes large amplitudes rotational oscillations about an axis

Table 4. *Bond lengths and e.s.d.'s*

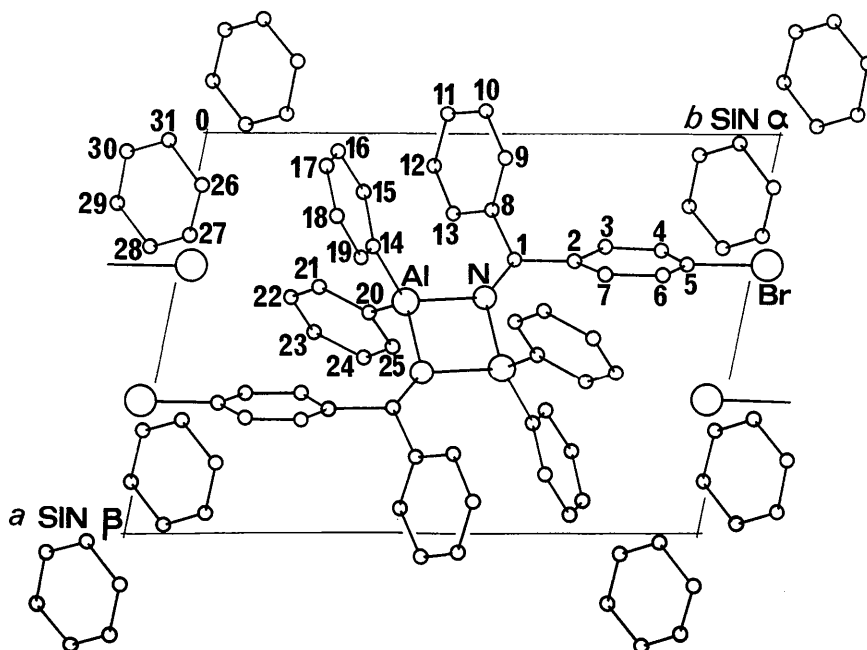| Al—N	1·916 (10) Å	C(2)–C(3)	1·429 (18) Å
Al—N′	1·918 (10)	C(3)–C(4)	1·377 (17)
Al—C(14)	1·979 (13)	C(4)–C(5)	1·430 (22)
Al—C(20)	1·956 (13)	C(5)–C(6)	1·336 (22)
N—C(1)	1·282 (15)	C(6)–C(7)	1·375 (18)
C(1)–C(2)	1·483 (16)	C(7)–C(2)	1·423 (19)
C(1)–C(8)	1·492 (16)	C(5)–Br	1·908 (14)
C(8)—C(9)	1·383 (18)	C(14)–C(15)	1·397 (17)
C(9)—C(10)	1·377 (21)	C(15)–C(16)	1·440 (21)
C(10)–C(11)	1·408 (27)	C(16)–C(17)	1·363 (25)
C(11)–C(12)	1·387 (24)	C(17)–C(18)	1·351 (21)
C(12)–C(13)	1·388 (21)	C(18)–C(19)	1·419 (22)
C(13)–C(8)	1·408 (18)	C(19)–C(14)	1·434 (19)
C(20)–C(21)	1·397 (16)	C(26)–C(27)	1·318 (38)
C(21)–C(22)	1·420 (20)	C(27)–C(28)	1·312 (38)
C(22)–C(23)	1·395 (22)	C(28)–C(29)	1·363 (44)
C(23)–C(24)	1·383 (21)	C(29)–C(30)	1·298 (46)
C(24)–C(25)	1·406 (20)	C(30)–C(31)	1·386 (41)
C(25)–C(20)	1·419 (18)	C(31)–C(32)	1·415 (37)

Fig. 1. Projection down [001].

Table 5. *Equations of the mean planes*

The equations are in the form $lX + mY + nZ = P$.

Atoms	*l*	*m*	*n*	*P*
Ten of Fig. 2	0·487	−0·029	−0·873	0·162
C(2) to C(7)	0·968	−0·038	−0·250	2·283
C(8) to C(13)	−0·027	0·761	−0·648	4·852
C(14) to C(19)	0·305	−0·912	−0·276	−3·751
C(20) to C(25)	−0·783	0·482	−0·395	−1·556
C(26) to C(31)	−0·133	0·617	−0·776	−1·846

normal to the plane of the ring. A simplified analysis shows that the observed U_{ij} are rather well reproduced by the assumption of a rigid body isotropic vibration of $T = 0·09$ Å^2 together with a libration about the ring axis of $\omega = 0·10$ radian^2, that is root mean square libration amplitude of about 18°. The appropriate correction to the bond lengths (Cruickshank, 1961) then increases the mean C–C bond length from 1·35 Å to 1·39 Å.

The benzene molecules occur in pairs related by the centre of symmetry at the origin. Viewed normal to the

planes of the rings, C(31) is almost directly above the centre of the C(30')–C(31') bond of the other ring, with C(31)–C(30') and C(31)–C(31') both equal to 3·75 Å. In addition, C(26)–C(30') = 3·88 Å. The perpendicular distance between the two rings is 3·69 Å.

I am grateful to the members of the Glasgow Crystallography group who have made available the KDF9 computer programs which were used in this work.

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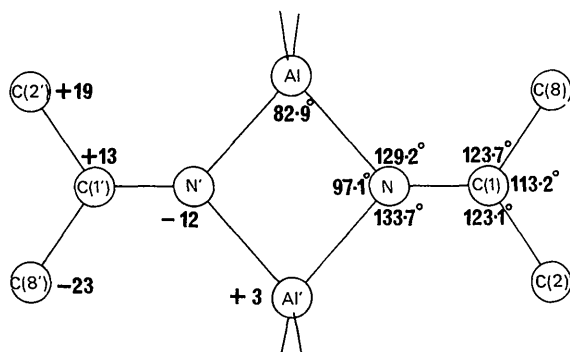WADE, K. & WYATT, B. K. (1967). *J. Chem. Soc.* (A), p. 1339.

Fig. 2. The planar central portion of the molecule. The figures on the left are the displacements, in thousandths of Å, from the weighted mean plane.